

Enhancement of polarization in a spin-orbit coupling quantum wire with a constriction

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We investigate the enhancement of spin polarization in a quantum wire in the presence of a constriction and a spin-orbit coupling segment. It is shown that the spin-filtering effect is significantly heightened in comparison with the configuration without the constriction. It is understood in the studies that the constriction structure plays a critical role in enhancing the spin filtering by means of confining the incident electrons to occupy one channel only while the outgoing electrons occupy two channels. The enhancement of spin-filtering has also been analyzed within the perturbation theory. Because the spin polarization arises mainly from the scattering between the constriction and the segment with spin-orbit coupling, the sub-band mixing induced by spin-orbit interaction in the scattering process and the interferences result in higher spin-filtering effect.

PACS numbers: 73.23.-b, 73.40.Gk

I. INTRODUCTION

The generation of a spin-polarized current in low dimensional semiconductor systems (LDSSs) has been studied extensively both for fundamental physics and for potential applications in spintronic devices¹. For these proposes the novel spintronic materials have been realized. Correspondingly, advanced electronic devices, such as spin transistors², spin waveguides³, spin filters⁴, etc., have been proposed. In narrow-gap semiconductor nanostructures such as InAs- and In_{1-x}Ga_xAs quantum wells, the inversion asymmetry of the confining potential due to the presence of the heterojunction⁵ results in the spin-orbit interaction (SOI), so that it leads to the spin splitting transport of the carriers in the absence of any applied magnetic field⁶. It is found that the SOI can be employed to generate the spin polarization in a T-shaped structure^{7,8} and a pure spin current in a Y-shaped junction⁹. The spin precession^{10,11,12} and spin Hall effect¹³ have been investigated in quantum wires with SOI. The studies of the spin-filtering effect in the wire in the presence of SOI show that the spin-filtering would not occur if the outgoing lead supports only one open channel^{14,15}. While for the wire with multi-channel, a finite transverse nonequilibrium spin polarization in leads¹⁶ is generated. The spatially averaged polarization density in the transverse direction is found to be in the third order of the SOI strength¹⁷.

In this work we propose a quantum wire system with a segment of SOI wire and a constriction to achieve an enhancement of spin polarization. We shall focus on the spin filtering effect, i.e., conductance spin polarization. Based on studies it is a challenge to enhance the spin polarization significantly in quantum wire systems in combination structure of a one-channel and a two-channel sections. It is found that the conductance spin polarization is very small if the constriction is absent. However, for the configuration of one channel occupied only in the constriction and two channels occupied in the segment with SOI, the spin-polarization reaches up to 95%. This

is interpreted by the fact that the higher polarization originates from the scattering of electrons at the interface between the constriction and the SOI segment wire. A perturbative analysis show that the contributions of the lowest two incoming channels to the spin-filtering always cancel each other partially. Therefore, the forbiddance of the second incoming channel by the constriction so that the interference effect between eigenstates of the SOI wire results in the effect of spin-filtering to be increased.

This paper is organized as follows. In Sec. II The structure of SOI quantum wire with a constriction is given. We then present the scattering-matrix formalism for the multimode spin-dependent transport. The numerical results of conductances and the conductance spin polarization are given In Sec. III. To understand the reason of enhancement of spin polarization, we analyze the effect of spin-filtering by means of the interference among the eigenstates of the SOI wire within a perturbative theory. Finally, a summary is given in the Sec. IV.

II. MODEL AND FORMALISM

Considering a two-dimensional electron gas (2DEG) formed in semiconductor heterostructures, its growth direction is along the y axis and 2DEG is in the x - z plane. In 2DEG a transverse hard wall potential is applied to form a quasi-one-dimensional (Q1D) quantum wire of width W_2 . We introduce a constriction of width W_1 and length L_1 in the wire as a schematic shown in Fig. 1. With the exception of the segment of length L_2 in the presence of the tunable^{19,20,21,22} spin-orbit coupling¹⁸, no SOI presents in remaining parts of the wire. The Hamiltonian is given by

$$\begin{aligned} H = & \frac{p_x^2 + p_z^2}{2m^*} + V(x, z) + \frac{\lambda(z)}{\hbar} p_x \sigma_z \\ & - \frac{1}{2\hbar} [\lambda(z) p_z \sigma_x + \sigma_x p_z \lambda(z)], \end{aligned} \quad (1)$$

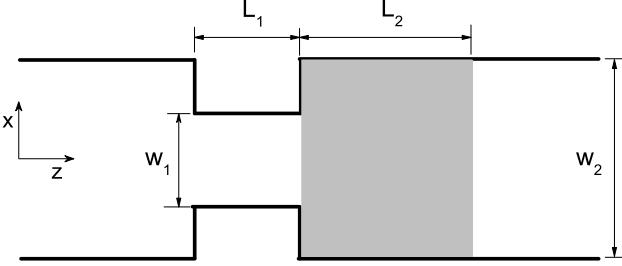


FIG. 1: Schematic illustration of a quantum wire with a SOI segment (shaded) and a constriction.

where m^* is the effective mass of electron, $\lambda(z)$ relates to Rashba coupling constant α through $\lambda(z) = \alpha[\Theta(z - z_0) - \Theta(z - z_0 - L_2)]$, and $V(x, z)$ is the confinement potential, i.e.,

$$V(x, z) = \begin{cases} 0 & |x| < W_1/2 \text{ (constriction), or } W_2/2 \text{ (wire)} \\ \infty & |x| \geq W_1/2 \text{ (constriction), or } W_2/2 \text{ (wire)} \end{cases} \quad (2)$$

The system can be solved by dividing it into several sections, i.e., the constriction, the segment in the presence of SOI, and the two semi-infinite wire. Considering the continuous conditions on the boundaries between sections, the scattering matrix formalism²³ can be built. Because of no SOI in two semi-infinite wires and the constriction, the solution of Shrödinger equations in these regions are plane waves with transverse modes due to the confinement in the x direction. For the segment with finite SOI, we need to consider the solution with spin-splitting due to the presence of SOI. To do this, we first introduce the dimensionless units: the coordinate $\mathbf{x} \rightarrow \mathbf{x}(W_2/\pi)$, the energy $E \rightarrow EE_0$ with $E_0 = \hbar^2\pi^2/(2m^*W_2^2)$, the wave vector $\mathbf{k} \rightarrow \mathbf{k}(\pi/W_2)$, and the SOI strength $\alpha \rightarrow \alpha\hbar^2\pi/(2m^*W_2)$. In the dimensionless unit, the Shrödinger equation for the segment with a finite SOI becomes

$$[k_x^2 + k_z^2 + \alpha(k_x\sigma_z - k_z\sigma_x)]\psi(x, z) = E\psi(x, z). \quad (3)$$

Its solution can be written in the form of $\psi(x, z) = \varphi(x)\exp(ik_z z)$, where $\varphi(x)$ satisfies the boundary condition $\varphi(\pi/2) = \varphi(-\pi/2) = 0$ due to a hard-wall potential described by Eq. (2) (the boundaries of wire described by the dimensionless values $\pm\pi/2$). In general, $\varphi(x)$ can temporarily be written in the form of $\varphi(x) = \xi_k \exp(ik_x x)$, where k_x is determined by the boundary condition and ξ_k is the spinor which is dependent on wave-vector. For a fixed energy E and a fixed longitudinal wave vector k_z , we can obtain four eigenvalues for k_x (k_1, k_2, k_3, k_4) from the relation $E = k_x^2 + k_z^2 \pm \alpha\sqrt{k_x^2 + k_z^2}$. The corresponding spinors are given by ξ_1, ξ_2, ξ_3 , and ξ_4 , respectively. Therefore,

$\varphi(x)$ can be expressed as a superposition of these four eigenfunctions,

$$\varphi(x) = c_1\xi_1 e^{ik_1 x} + c_2\xi_2 e^{ik_2 x} + c_3\xi_3 e^{ik_3 x} + c_4\xi_4 e^{ik_4 x}, \quad (4)$$

where c_1, c_2, c_3 , and c_4 are coefficients. With the help of the boundary conditions at the edges $x = \pm\pi/2$, we can, in principle, obtain the dispersion relation of electron, $E = E(k_z)$, in the wire with the presence of the SOI. $E(k_z)$ can only be obtained numerically. Due to the time-reversal symmetry of the system¹⁵, the dispersion relation $E(k_z)$ has the symmetry of k_z and $-k_z$. For a fixed value of k_z the coefficients c_1, c_2, c_3 , and c_4 can be obtained by the boundary conditions. Because of finite width of wire, the transverse modes exist for the electrons in the wire. In order to reveal possible transport channels, we use n describes the transverse mode. Correspondingly, the wave-vector k_z can be written in the form as $k_z(n, \sigma)$. For example, the analytic relation of energy can be perturbatively obtained as $E_{n,\sigma}(k_z) \approx n^2 + k_z^2 + \sigma\alpha k_z - \alpha^2/4$, where $\sigma = \pm$. Thus a complete set of eigenfunctions for the quantum wire in the presence of the SOI is found to be

$$\varphi_{n\sigma}(x)e^{ik_z(n,\sigma)x} \text{ and } \tilde{\varphi}_{n\sigma}(x)e^{-ik_z(n,\sigma)x}. \quad (5)$$

It is need to emphasize that the transverse mode n and spin σ are not good quantum numbers. We adopt them as indices only for the eigenfunctions obtained by numerical calculations. Generally, the eigenfunctions include the mixing of all the transverse modes of the wire without SOI. In Section III, the perturbation theory will indicate that the mixing among the transverse modes results in the spin-filtering effect. In addition, the time-reversal symmetry implies that the right-going and left-going electrons have anti-parallel spins. This leads to $\varphi_{n\sigma}(x) \neq \tilde{\varphi}_{n\sigma}(x)$.

After obtaining the sets of eigenfunctions for all four sections, the scattering matrices can be obtained according to the multimode scattering-matrix procedure²³. In the left (right) semi-infinite wire without SOI, the wave function can be written in the form as

$$\psi(x, z) = \sum_{n\sigma} \varphi_1^{n\sigma} \left(a_{n\sigma}^{L(R)} e^{ik_1(n,\sigma)z} + b_{n\sigma}^{L(R)} e^{-ik_1(n,\sigma)z} \right), \quad (6)$$

where $k_1(n,+) = k_1(n,-) = \sqrt{E - n^2}$, and $\varphi_1^{n\sigma} = \sqrt{2/\pi} \sin[n(x + \pi/2)] |\sigma\rangle_z$ with spinors $|+\rangle_z = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $|-\rangle_z = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$. In the constriction, the wave function takes the form as

$$\psi(x, z) = \sum_{n\sigma} \varphi_c^{n\sigma} \left(a_{n\sigma}^c e^{ik_c(n,\sigma)z} + b_{n\sigma}^c e^{-ik_c(n,\sigma)z} \right), \quad (7)$$

where $\varphi_c^{n\sigma} = \sqrt{2/\pi r} \sin[n(x + \pi r/2)/r] |\sigma\rangle_z$ with $r = W_1/W_2$, and $k_c(n,+) = k_c(n,-) = \sqrt{E - n^2/r^2}$. In the segment with a finite SOI, the wave function is given by

$$\psi(x, z) = \sum_{n\sigma} \left(a_{n\sigma} \varphi_2^{n\sigma} e^{ik_2(n,\sigma)z} + b_{n\sigma} \tilde{\varphi}_2^{n\sigma} e^{-ik_2(n,\sigma)z} \right). \quad (8)$$

The scattering-matrices can be obtained by considering the boundary conditions at interfaces, i.e., the continuity of the wavefunctions and the step change of their derivatives crossing the interfaces. The step change of the derivatives of wavefunctions comes from the step change of the strength of SOI²⁴ in the wire. For example, at the interface of the constriction and the SOI segment, localized at $z = z_0$, we have $\psi'(x, z_0 + 0_+) - \psi'(x, z_0 - 0_+) = (i\alpha/2)\sigma_x\psi(x, z_0)$. Combining all the scattering-matrices for all waveguide sections²³, the total scattering-matrix connects outgoing amplitudes $\{b_{n_L\sigma_L}^L\}$ and $\{a_{n_R\sigma_R}^R\}$ to the incoming amplitudes $\{a_{n_L\sigma_L}'^L\}$ and $\{b_{n_R\sigma_R}'^R\}$, i.e.,

$$\begin{pmatrix} b_{n_L\sigma_L}^L \\ a_{n_R\sigma_R}^R \end{pmatrix} = \begin{pmatrix} r_{n_L\sigma_L, n_L'\sigma_L'} & t_{n_L\sigma_L, n_R'\sigma_R'}' \\ t_{n_R\sigma_R, n_L'\sigma_L'} & r_{n_R\sigma_R, n_R'\sigma_R'}' \end{pmatrix} \begin{pmatrix} a_{n_L'\sigma_L'}^L \\ b_{n_R'\sigma_R'}^R \end{pmatrix}, \quad (9)$$

where the Einstein's sum rule is adopted and the summation should be taken over propagating modes in the left (right) semi-infinite wires¹⁵ only. All these propagating modes are normalized with their velocities. The spin-dependent conductance at zero temperature is given by summing over the transmission modes²⁵,

$$G_{\sigma_L\sigma_R} = \frac{e^2}{h} \sum_{n_L n_R} |t_{n_R\sigma_R, n_L\sigma_L}|^2. \quad (10)$$

From this formula, we define the total conductance $G_\uparrow = G_{\uparrow\uparrow} + G_{\uparrow\downarrow}$ for the spin-up incident electrons, while $G_\downarrow = G_{\downarrow\uparrow} + G_{\downarrow\downarrow}$ for spin-down incident electrons. The total conductance of non-polarized incident electrons is given by $G = G_\uparrow + G_\downarrow$.

The spin polarization after the electrons transporting through the system (so-called conductance spin polarization) can be expressed in terms of the scattering matrix¹⁵:

$$\begin{aligned} P_x + iP_y &= \frac{2e^2/h}{G} \sum_{n_R, n_L \sigma_L} t_{n_R\uparrow, n_L\sigma_L}^* t_{n_R\downarrow, n_L\sigma_L}, \\ P_z &= \frac{(G_{\uparrow\uparrow} + G_{\uparrow\downarrow}) - (G_{\downarrow\uparrow} + G_{\downarrow\downarrow})}{G}. \end{aligned} \quad (11)$$

Moreover, because only x -component of the conductance spin polarization P_x is nonzero in present system configuration, we are concerned with the spin related conductance with respect to the x direction. The conductances of "spin-up" and "spin-down" transmitted electrons with respect to the x direction can be expressed as

$$\begin{aligned} G_{\sigma_x}^+ &= \frac{e^2}{2h} \sum_{n_R, n_L \sigma_L} |t_{n_R\uparrow, n_L\sigma_L} + t_{n_R\downarrow, n_L\sigma_L}|^2, \\ G_{\sigma_x}^- &= \frac{e^2}{2h} \sum_{n_R, n_L \sigma_L} |t_{n_R\uparrow, n_L\sigma_L} - t_{n_R\downarrow, n_L\sigma_L}|^2. \end{aligned} \quad (12)$$

Therefore, the total conductance G satisfies $G = G_{\sigma_x}^+ + G_{\sigma_x}^-$ and P_x can be defined as

$$P_x = \frac{G_{\sigma_x}^+ - G_{\sigma_x}^-}{G_{\sigma_x}^+ + G_{\sigma_x}^-}, \quad (13)$$

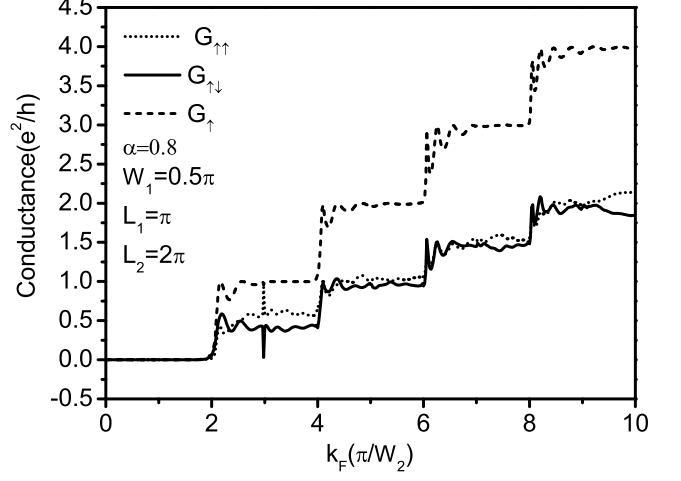


FIG. 2: Spin resolved conductances $G_{\uparrow\uparrow}$, $G_{\uparrow\downarrow}$, and $G_{\downarrow\uparrow}$ as functions of Fermi wave vector of incident electrons $k_F = \sqrt{E_F}$. The parameters are chosen as (corresponding to $W_2 = \pi$): $\alpha = 0.8$, $W_1 = 0.5\pi$, $L_1 = \pi$, and $L_2 = 2\pi$.

which is consistent with Eq. (11). In the next section, we will perform the numerical calculation and the results show a significant enhancement of the x component of conductance spin polarization.

III. RESULTS AND DISCUSSION

In this section we present the numerical calculations of the conductance and its spin-polarized components. The spin-filtering will be analyzed in the perturbation theory. In the numerical calculation, the following parameters are used: $W_2 = 100$ nm, $m^* = 0.036m_e$, $E_0 \approx 1.04$ meV, and $\alpha_0 = \hbar^2\pi/(2m^*W_2) = 3.32 \times 10^{-11}$ eVm.

The conductances $G_{\uparrow\uparrow}$, $G_{\uparrow\downarrow}$, and $G_{\downarrow\uparrow}$ as functions of Fermi wave vector of incident electrons k_F are shown in Fig. 2, where $k_F = \sqrt{E_F}$ with E_F the dimensionless Fermi energy. As it is expected, the total conductance G_\uparrow is quantized. The appearance of plateaus corresponds to the energy sweeping over a new channel supplied by the constriction. The resonant structures near of the edges of steps come from the multi-reflection between the two ends of the constriction^{26,27}. In comparison to G_\uparrow , its spin-polarized components $G_{\uparrow\uparrow}$ and $G_{\uparrow\downarrow}$ exhibit more resonant structures because the Rashba SOI induces the spin splitting and results in a subband intermixing¹⁰. At the energy near to the bottom of the third subband $k_F \approx 3$, the spin conductances exhibit a sharp peak for $G_{\uparrow\uparrow}$ and a sharp dip for $G_{\uparrow\downarrow}$. This phenomena is related to the details of the spin-dependent scattering mechanism of electron transport through the whole system configuration.

In order to show the spin-filtering effect, we calculated the spin-polarized components of conductance spin po-

larization. Fig. 3(a) shows the components $G_{\sigma_x}^+$, $G_{\sigma_x}^-$, and the total conductance G . The conductance spin polarization P_x , P_y , and P_z as functions of Fermi wave vector of incident electrons are shown in Fig. 3(b). It is seen that if the length of the constriction is chosen to be $L_1 = 0.5\pi = W_1$, the plot of the total conductance G becomes relatively smooth. The reason is that both the amplitude and the frequency of oscillation depend on the aspect ratio of the constriction²⁷. In Fig. 3(b), it is found that a large transverse conductance spin polarization P_x can be achieved. The enhancement reaches the strongest in the situation when the constriction is narrow enough to supply one channel only and the SOI segment supplies two channels, *i.e.*, in the range $2 < k_F < 3$. P_y and P_z are always vanished because of the symmetry $V(x, z) = V(-x, z)$ and the time-reversal symmetry¹⁵ in the system.

In order to understand how large polarization is generated in this structure, we analyze the origin of spin-filtering effect in the perturbation theory. To do this we assume that the SOI is weak and solve the eigenfunctions of the SOI wire perturbatively. The Hamiltonian for the SOI segment of wire can be divided into two parts,

$$H_0 = k_x^2 + k_z^2 + V(x) - \alpha k_z \sigma_x \quad (14)$$

and

$$H_1 = \alpha k_x \sigma_z. \quad (15)$$

We then treat H_1 as a perturbation. The eigenvalues of H_0 are found to be $E_{n\pm}^{(0)} = n^2 + k_z^2 \mp \alpha k_z$ and corresponding eigenfunctions are

$$\varphi_{n\pm}^{(0)}(k_z, x) = \phi_{n\pm}^{(0)} e^{ik_z z}, \quad (16)$$

where $\phi_{n\pm}^{(0)} = \sqrt{2/L\pi} \sin[n(x + \pi/2)]$ with n the transverse subband index, $|+\rangle_x = (1/\sqrt{2}) \begin{pmatrix} 1 \\ 1 \end{pmatrix}$ and $|-\rangle_x = (1/\sqrt{2}) \begin{pmatrix} 1 \\ -1 \end{pmatrix}$ with \pm the spin index, and L is the length of the SOI segment. The relevant matrix elements of the perturbation H_1 are found as

$$\begin{aligned} \langle \varphi_{m\mp}^{(0)} | H_1 | \varphi_{n\pm}^{(0)} \rangle &= i(\alpha/\pi) [2nm/(n^2 - m^2)] \\ &\quad [1 - (-1)^{n+m}] \delta_{k_z, k_z'} \end{aligned} \quad (17)$$

and other matrix elements are zero. The perturbative eigenfunction up to the second order in H_1 is given by

$$\varphi_{n\pm} = \varphi_{n\pm}^{(0)} + \frac{\alpha^2}{\pi^2} \sum'_{m,l} \frac{4nm}{(n^2 - m^2)^4} \left[\frac{2nm\varphi_{n\pm}^{(0)}}{(1 \mp \frac{2\alpha k_z}{n^2 - m^2})^2} + i\frac{\pi}{\alpha} \frac{(n^2 - m^2)^2 \varphi_{m\mp}^{(0)}}{(1 \mp \frac{2\alpha k_z}{n^2 - m^2})} + \frac{4ml(n^2 - m^2)^2 \varphi_{l\pm}^{(0)}}{(1 \mp \frac{2\alpha k_z}{n^2 - m^2})(n^2 - l^2)(l^2 - m^2)} \right], \quad (18)$$

where the sum extends over the positive integers and m is of opposite parity with n , l is of the same parity as n but $n \neq l$.

Using these wavefunctions we can calculate the x -component of the spin polarization density. Because the wavefunction of a right-going electron with definite Fermi energy in the SOI segment can be written as (assume that only the lowest two channels are open) $\psi(z) = \sum_{i=1,2} \sum_{\sigma=\pm} a_{i\sigma} \phi_{i\sigma} e^{ik_{i\sigma} z}$. For simplicity, we ignore the reflection at the interface between the SOI segment and the right semi-infinite wire. The x -component of the spin polarization density in the SOI segment is defined as, $P_x(x, z) = \langle \psi(x', z') | \delta(x - x') \delta(z - z') \sigma_x | \psi(x', z') \rangle$. It is found

$$P_x(x, z) = \text{Re} \sum_{i,j=1,2} \sum_{\sigma,\sigma'=\pm} (a_{i\sigma}^* a_{j\sigma'} \phi_{i\sigma}^\dagger \sigma_x \phi_{j\sigma'} e^{-i(k_{i\sigma} - k_{j\sigma'})z}).$$

Let us consider an incident electron in the constriction with one open channel. Because no SOI, the wave function can be written as $\psi(z) = a'_{1+} \phi_{1+}^{(0)} e^{ik_1 z} + a'_{1-} \phi_{1-}^{(0)} e^{ik_1 z}$. Due to $V(x, z) = V(-x, z)$, the operator $\sigma_x R_x$ commutes with the Hamiltonian, where R_x is the reflection transformation with respect to the x axis¹⁵. $\varphi_{1+}^{(0)}$,

φ_{1+} , and φ_{2-} are eigenstates of $\sigma_x R_x$ with the eigenvalue 1. The state $\varphi_{1+}^{(0)}$ can only be scattered to φ_{1+} and φ_{2-} . Similarly, the state $\varphi_{1-}^{(0)}$ can only be scattered to φ_{1-} and φ_{2+} with the eigenvalue -1. In the Landau-Büttiker formalism, the conductance is independent of phases of the incident waves in incoming channels. The phase of a'_{1+} is independent of that of a'_{1-} . Therefore, the phases of a_{1+} and a_{2-} , which are transferred from a'_{1+} , have no relation with those of a_{1-} and a_{2+} , transferred from a'_{1-} . Under the phase average, the terms $\text{Re} [a_{i\sigma}^* a_{j\sigma'} \phi_{i\sigma}^\dagger \sigma_x \phi_{j\sigma'} e^{-i(k_{i\sigma} - k_{j\sigma'})z}]$ vanish if $i = j$ and $\sigma \neq \sigma'$, or $i \neq j$ and $\sigma = \sigma'$.

After taking away those vanished terms under the phase average, the remained terms in $P_x(x, z)$ can be divided into two kinds, *i.e.*, the contributions from each single state,

$$P_x^s(x, z) = \sum_{i=1,2} \sum_{\sigma=\pm} |a_{i\sigma}|^2 \phi_{i\sigma}^\dagger \sigma_x \phi_{i\sigma} \quad (19)$$

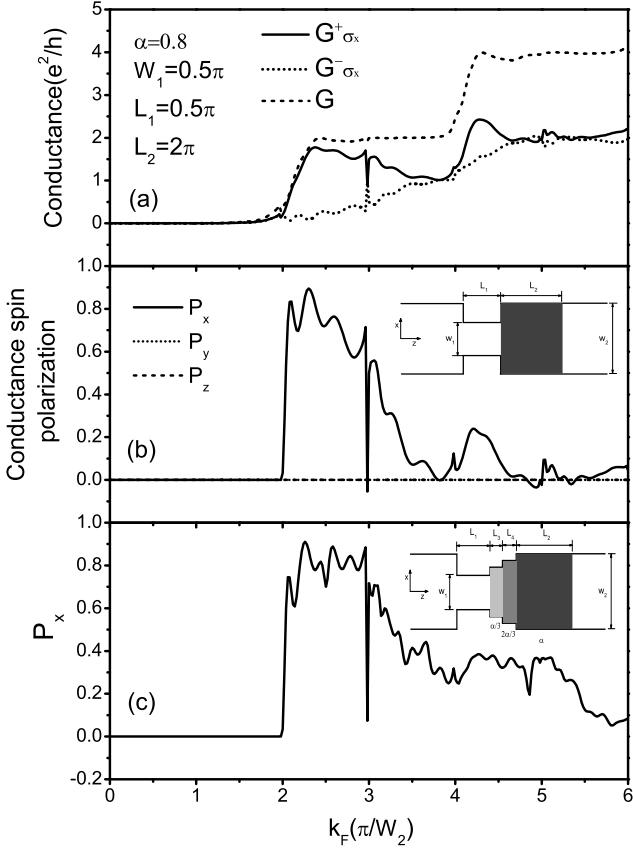


FIG. 3: (a) Spin resolved conductances $G_{\sigma_x}^+$ and $G_{\sigma_x}^-$, and total conductance G ; (b) The conductance spin polarization P_x , P_y , and P_z as a function of Fermi wave vector of incident electrons. The parameters are chosen as: $\alpha = 0.8$, $W_1 = 0.5\pi$, $L_1 = 0.5\pi$, $L_2 = 2\pi$. (c) P_x in the case of sequentially increasing widths and SOI strengths between the constriction and the SOI segment. The boundary between the constriction and the SOI segment is smoothed by adding two short segments with sequentially increasing widths $2\pi/3$, $5\pi/6$ and SOI strengths $0.8/3$, $1.6/3$. The lengths of these two sections are π (as seen in the inset). The other parameters are the same as those in (b).

and the contributions from the interference,

$$P_x^i(x, z) = \sum_{i,j=1,2} \sum_{\sigma=\pm} \text{Re} \left[a_{i\sigma}^* a_{j\bar{\sigma}} \phi_{i\sigma}^\dagger \sigma_x \phi_{j\bar{\sigma}} e^{-i(k_{i\sigma} - k_{j\bar{\sigma}})z} \right]. \quad (20)$$

Using Eq. (18) and integrating over the transverse section of the wire, we find $\sum_{\sigma=\pm} \int_{-\pi/2}^{\pi/2} \phi_{i\sigma}^\dagger \sigma_x \phi_{i\sigma} dx = 0 + O(\alpha^3)$ ($i = 1$ and 2). In addition, the dependence of the transmission amplitudes on α is found as follows: $a_{1+} = [c_1 + c_2 \alpha^2 + O(\alpha^3)] a'_{1+}$, $a_{2-} = [c_3 \alpha + O(\alpha^3)] a'_{1+}$, $a_{1-} = [c_1 + c_4 \alpha^2 + O(\alpha^3)] a'_{1-}$, and $a_{2+} = [c_5 \alpha + O(\alpha^3)] a'_{1-}$, where c_1, c_2, \dots, c_5 are coefficients determined by the boundary conditions of the wavefunctions. Therefore, the difference between

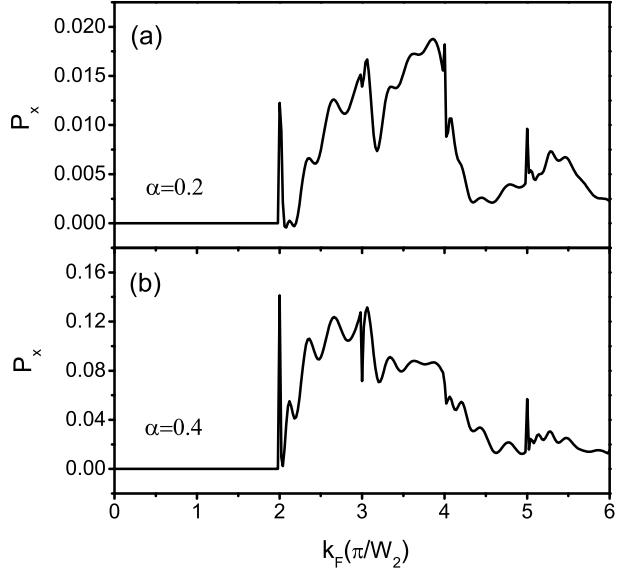


FIG. 4: Conductance spin polarization for two different values of SOI strength: $\alpha = 0.2$ and 0.4 . The other parameters are the same as those in Fig. 3.

$|a_{1+}|^2$ ($|a_{2+}|^2$) and $|a_{1-}|^2$ ($|a_{2-}|^2$) is in order of α^2 . Thus, the contribution from the single state, $P_x^s(z) = \int_{-\pi/2}^{\pi/2} P_x^s(x, z) dx$, is in order of α^2 . For those terms contributed from the interference $P_x^i(x, z)$, to the first order, we have $\int_{-\pi/2}^{\pi/2} \phi_{1+}^\dagger \sigma_x \phi_{2-} dx = i\alpha 16/[3\pi(3+2\alpha k_z)]$ and $\int_{-\pi/2}^{\pi/2} \phi_{1-}^\dagger \sigma_x \phi_{2+} dx = -i\alpha 16/[3\pi(3-2\alpha k_z)]$. Therefore, the contribution from the interference $P_x^i(x, z)$ is also in order of α^2 . As a result, the total polarization $P_x(z)$ is in order of α^2 . In comparison to the results in an infinite SOI wire¹⁷ without scattering, where the polarization is in the order of α^3 , the α^2 -dependence of $P_x(z)$ in our wire configuration with a constriction arises from the interface scatterings. The conductance spin polarizations on different strength of Rashba SOI are shown in Fig. 4.

In order to understand a critical role of the constriction for the appearance of a higher spin polarization in this system configuration. We examine $P_x^s(z)$ and $P_x^i(z)$ separately. For simplicity, we only considered the subband intermixing among four states $\varphi_{1+}^{(0)}$, $\varphi_{1-}^{(0)}$, $\varphi_{2+}^{(0)}$, and $\varphi_{2-}^{(0)}$ induced by the perturbation H_1 . Actually, the intermixing among these four states plays the main role in achieving a large polarization. For $k_z > 0$, the form of the perturbed wavefunctions indicates that the distortion of φ_{1-} and φ_{2+} from $\varphi_{1-}^{(0)}$ and $\varphi_{2+}^{(0)}$ is greater than that of φ_{1+} and φ_{2-} from $\varphi_{1+}^{(0)}$ and $\varphi_{2-}^{(0)}$. Therefore, the state $\varphi_{1+}^{(0)}$ is more likely to be scattered into the state φ_{1+} than the state $\varphi_{1-}^{(0)}$ to be scattered into φ_{1-} . The probability of $\varphi_{1+}^{(0)}$ being scattered into the state φ_{2-} is smaller than that of $\varphi_{1-}^{(0)}$ into φ_{2+} . Namely, $|a_{1+}|^2$ is larger than

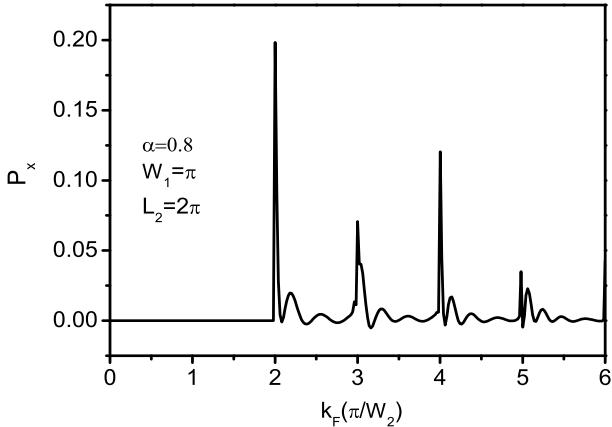


FIG. 5: Conductance spin polarization for a configuration without the constriction ($W_1 = W_2$). The other parameters are the same as those in Fig. 3.

$|a_{1-}|^2$ and $|a_{2+}|^2$ is larger than $|a_{2-}|^2$. The term $P_x^s(z)$ is positive. However, if there is no the constriction to confine the electron to the lowest channel, the incident electron can occupy two channels in the left semi-infinite wire. According to the above analysis, the lowest channel (the states $\varphi_{1+}^{(0)}$ and $\varphi_{1-}^{(0)}$) gives a positive contribution to $P_x^s(z)$, but the second channel (the states $\varphi_{2+}^{(0)}$ and $\varphi_{2-}^{(0)}$) will give a negative contribution to $P_x^s(z)$. Therefore, the polarization is reduced due to the contributions of two channels being cancelled partially. Besides, when two channels are occupied by incident electrons, the interference term $P_x^i(z)$ will be also reduced. For the case without the constriction, the polarization is plotted in Fig. 5. It is shown that the polarization is small and nonzero only when the right lead supplies at least two channels¹⁵. However, the polarization would be enhanced if there is a constriction which supplies one channel in the region of constriction and two channels in the SOI segment(four subbands if spin indexes are counted). The simplest structure is the width of constriction to be half of the width of wire $W_1 = 0.5W_2$.

Since the above discussion is for $k_z > 0$, i.e., for right-going electrons, the main contribution to $P_x^i(z)$ comes from the interference between states φ_{1-} and φ_{2+} . Eq. (20) shows that this interference oscillates with the longitudinal length in z . The period of the oscillation is $2\pi/(k_{1-} - k_{2+})$. The oscillation of the polarization P_x along with the length of the SOI segment is plotted in Fig. 6(a). In the numerical calculations the Fermi wave vector is taken $k_F = 2.301$, so we have $k_{1-} \approx 1.890$ and $k_{2+} \approx 1.488$. Therefore, the period of the oscillation is 4.975π . The structure of the oscillation with other periods is caused by the interference between φ_{1+} and φ_{2-} , and the reflection amplitudes from the right interface of the SOI segment, which can be seen in the Fourier spectrum Fig. 6(b). For different lengths of the SOI wire,

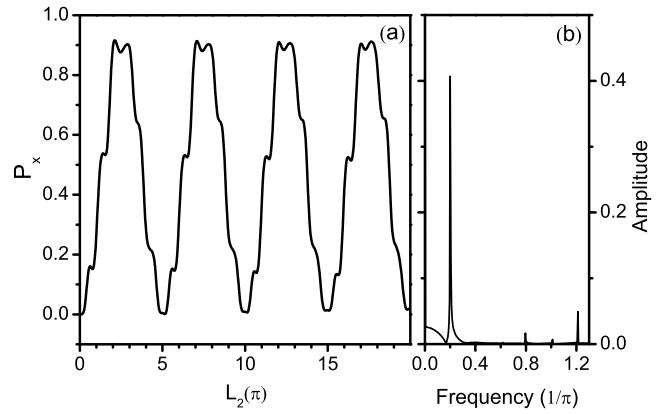


FIG. 6: (a) The oscillation of conductance spin polarization along the SOI segment and (b) the corresponding Fourier frequency spectrum, where the Fermi wave vector is fixed at $k_F = 2.301$. The other parameters are the same as those in Fig. 3.

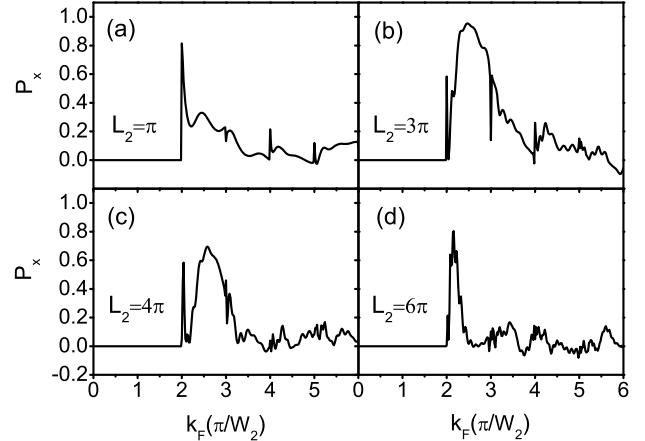


FIG. 7: Conductance spin polarizations for different lengths of the SOI segment: $L_2 = \pi$, 3π , 4π , and 6π . The other parameters are the same as those in Fig. 3.

the conductance spin polarizations as functions of Fermi wave vector have been shown in Fig. 7. The numerical results show that the polarization is sensitive to the length of the SOI segment. Especially, when $L_2 = 3\pi$, the large spin polarization may be kept over a wide range of incident energy.

The above calculations show the effect of the length of SOI segment on the spin polarization. The width of SOI segment is influential in the generation of higher spin polarization. Let us look at the dimensionless form of Hamiltonian first, the dimensionless coefficient of SOI takes the form as $2m^*W_2\alpha/(\hbar^2\pi)$ and the energy takes the form as $2m^*W_2^2E/(\hbar^2\pi^2)$, where W_2 is the width of the wire. From these we see that the dimensionless values of the SOI strength and the energy are proportional to

W_2 and W_2^2 , respectively. In the dimensionless formalism, the transport of an electron with energy E through a quantum wire of width W_2 with the SOI strength α is entirely equivalent with that of an electron with energy $\gamma^{-2}E$ through a wire of width γW_2 with the SOI strength $\gamma^{-1}\alpha$, where γ is an arbitrary real number. If the SOI segment is widened ($\gamma > 1$) from the width W_2 to γW_2 and the energy of indicant electrons is decreased from E to $\gamma^{-2}E$, but the SOI strength α is retained unchanged, the only change is the dimensionless SOI strength is increased from α to $\gamma\alpha$ in the dimensionless formalism. In another word, when we widen the wire from W_2 to γW_2 , keeping the SOI strength unchanged is equivalent to heighten the dimensionless SOI strength γ times if the energy of indicant electrons is reduced to $\gamma^{-2}E$ so that the dimensionless energy does not change. The net effect is to augment the SOI in the region of segment and leads to enhance the spin polarization. This effect can be understood qualitatively in another way. As known that the spaces between the discrete energy levels become small when the width of the wire increases, so that the contribution from the SOI is increased. Then, the sub-band mixing becomes stronger. If we decrease the energy of incident electrons correspondingly so that scattering from one-channel to two-channel is retained, the higher polarization is generated.

Although the sharp boundary conditions in the geometry of system configuration and in the strength of SOI have been considered in our calculations, both the effect of spin filtering and its enhancement should be robust and not sensitive to the specific choice of boundary condition if only a constriction and a SOI segment are presented. To be compared we smooth the boundary by adding two short segments with sequentially increasing widths and SOI strengths between the constriction and the SOI segment. The numerical results provide the evidences that the amplitude of the spin polarization is almost unchanged (see Fig. 3(c)). Only change is the resonant structure. The boundary for the wire only decides the resonant structure of the conductance spin polarization, which could be seen in our perturbative analysis, but not reduce the spin-filtering effect significantly. In essence, the spin polarization arises from the distortion of the transverse wavefunction of the SOI segment $\varphi_{n\sigma}(x)$ from the wavefunction of the wire without SOI $\varphi_{n\sigma}^{(0)}(x)$ due to the sub-band mixing. The enhancement of the spin-filtering is less dependent of the boundary. The alpha-squared scaling for the strength of spin filtering does remain even in cases with gradual changed boundaries. Differing an width uniform wire in the presence of a SOI section, in which the contributions of the lowest two incoming channels to the polarization of the transmitted

current always cancel each other partially, it is evident that the interference and the scattering in the present configuration, due to the configuration of a constriction confining the incident electrons to occupy one channel only while the outgoing electrons occupy two channels, increase the spin polarization significantly.

IV. CONCLUDING REMARKS

In summary, we have investigated numerically the spin-filtering in a quantum wire with a constriction and a SOI segment. The results show a higher conductance spin polarization generated in the transverse direction in comparison to configuration without the constriction. The spin polarization has been analyzed with the scattering processes and the perturbation theory. It is found that the enhancement is mainly due to the presence of a constriction which confines the incident electrons to occupy only one channel. The significant spin-filtering occurs when the constriction supplies one channel and the SOI wire supplies two channels. The spin-filtering mainly arises from the scattering between the constriction and the SOI segment. The sub-band mixing effect and the interference of different spin-states induced by the SOI segment dominate the spin-filtering effect in the scattering process. In addition, in contrast to that the polarization is in the third order of α for a uniform wire, the induced conductance spin polarization in present system configuration is in the second order of α . The predication of a higher spin-filtering effect in present configuration is able to be observed experimentally. The studies have been extended to the case of gradual change in space between the constriction and the SOI segment. It is shown that a higher spin-filtering occurs also if only the constriction supplies one channel and the SOI wire supplies two channels.

Although the present paper only consider the Rashba SOI, the significant effect of spin-filtering in the longitudinal direction instead of in the transverse direction can be retained if the linear Dresselhaus SOI is utilized instead of the Rashba SOI. However, the spin-filtering will be reduced if both Rashba and Dresselhaus SOI are presented. The spin-filtering vanishes if two kinds of SOI have the same strength. The reason is that the dispersion relation becomes rigorously parabolic again and the sub-band mixing disappears.

Acknowledgments

This work is supported by RFDP-China, NNSF-China No. 10674004, and NBRP-China No. 2006CB921803.

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